ROH +
$$CS_2$$
 + MeI $\xrightarrow{n-Bu_4NHSO_4}$ RO-C-SMe $\frac{0}{50\% \text{ aq. NaOH}}$ RO-C-SMe

Scheme 1

Scheme 2

4a: R₁ = H 4b: R₁ = Me 4c: R₁ = OMe

5a: R₁ = H (77%) **5b**: R₁ = Me (83%) **5c**: R₁ = OMe (85%)

6a: R₁ = H (88%) 6b: R₁ = Me (93%) 6c: R₁ = OMe (81%)

Scheme 3. Reagents: (a) resorcinol, BF₃-OEt₂, 100°C, 2h; (b) PPh₃, DIAD, MeOH, THF, rt, 5 min.; (c) CS₂, R₂X, n-Bu₄N•HSO₄, aq. NaOH, THF, rt, 3-7 h.

Scheme 4. Reagents: CS₂, R₂X, n-Bu₄N•HSO₄, aq. NaOH, THF, rt, 3 h.

MeO OH MeO
$$R_1$$

MeO R_1

MeO R_1

MeO R_1

MeO R_1

MeO R_2

MeO R_1

MeO R_1

MeO R_2

MeO R_1

MeO R_2

MeO R_1

MeO R_2

MeO R_1

MeO R_2

MeO R_2

MeO R_1

MeO R_2

MeO R_2

MeO R_1

MeO R_2

MeO R_2

MeO R_3

MeO R_4

MeO

Scheme 5. Reagents: CS₂, R₂X, n-Bu₄N•HSO₄, aq. NaOH, THF, rt, 3-7 h.

Dose Response Studies in MCF-7 Cells

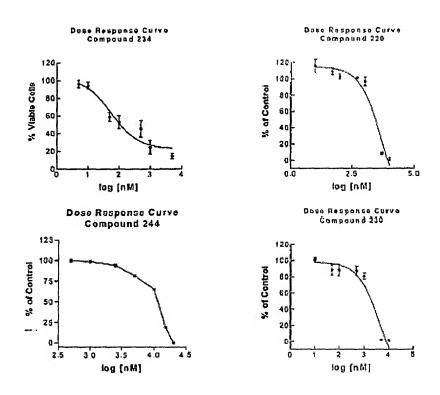
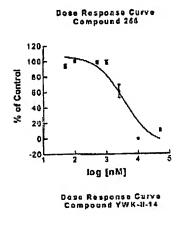
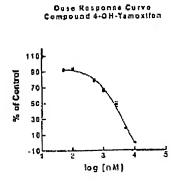


FIGURE 6

Dose Response Studies in MCF-7 Cells





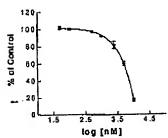
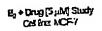


FIGURE 7

Screening Data for Isoflavone Library In MCF-7 (ER+) Cells in the presence of Estradiol



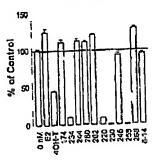


FIGURE 8

Screening Data for Isoflavone Library in MDA-MB-231 (ER-) Cells

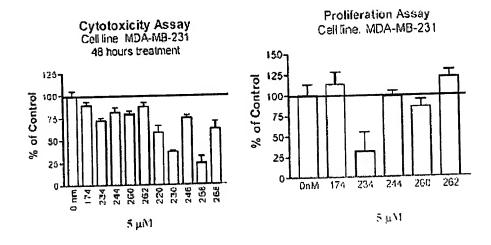


FIGURE 9

306a: R₁=H, R₂=OMe 306b: R₁=Me, R₂=OMe 306c: R₁=OMe, R₂=OMe 306d: R₁=H, R₂=OBn 306f: R₁=OMe, R₂=OBn 308a: X=S, R₁=OMe, R₂=OBn (96%) 308b: X=O, R₁=OMe, R₂=OBn (93%) 308c: X=S, R₁=H, R₂=OMe (90%) 308d: X=S, R₁=Me, R₂=OMe (83%) 308e: X=S, R₁=OMe, R₂=OMe (94%) 308f: X=S, R₁=H, R₂=OBn (91%) 309a: X=S, R₁=OMe, R₂=OBn (83%) 309b: X=O, R₁=OMe, R₂=OBn (89%) 309c: X=S, R₁=H, R₂=OMe (84%) 309d: X=S, R₁=Me, R₂=OMe (73%) 309e: X=S, R₁=OMe, R₂=OMe (78%)

 $\begin{array}{c} \text{Et}_2\text{OBF}_3,\,\text{Me}_2\text{S}\,\,(\text{for 311a})\\ \text{H}_4\text{NCO}_2,\,\text{Pd/C},\,\text{MeOH}\,\,(\text{for 311b})\\ \text{BBr}_3,\,\text{CH}_2\text{Cl}_2\,\,(\text{for 311c-f}) \end{array}$

 $\begin{array}{c} \text{Et}_2\text{OBF}_3\text{, Me}_2\text{S (for 310a)} \\ \text{H}_4\text{NCO}_2\text{, Pd/C, MeOH (for 310b)} \\ \text{BBr}_3\text{, CH}_2\text{Cl}_2\text{ (for 310c-f)} \end{array}$

311a: X=S, R₁=OMe (89%) 311b: X=O, R₁=OMe (88%) 311c: X=S, R₁=OH (83%) 311d: X=O, R₁=OH (75%) 311e: X=S, R₁=H (78%) 311f: X=S, R₁=Me (73%)

310a: X=S, R₁=OMe (86%) 310b: X=O, R₁=OMe (87%) 310c: X=S, R₁=OH (93%) 310d: X=O, R₁=OH (92%) 310e: X=S, R₁=H (85%) 310f: X=S, R₁=Me (81%)